Mathmatial Foundations of Reinforcement Learning

Linear function approximation

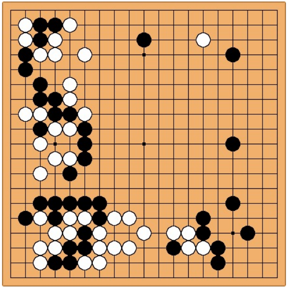
Yuting Wei

Statistics & Data Science, Wharton
University of Pennsylvania

Fall 2023

Outline

Humungous state space



$$S \approx 2 \cdot 10^{170}$$

Exploiting **low-complexity model** is essential for efficient RL!

- Save computation/space/data
- Generalize across state or states and actions

Function approximation

Function approximation

The *object of interest* possesses some *low-dimensional representation*.

- value function
- Q-function
- transition kernel
- reward
- policy

- Parametric:
  - Linear combinations of features
  - Neural networks
- Nonparametric:
  - Decision trees
  - Nearest neighbors

We will focus on *differentiable* function approximation and apply first-order methods to *incrementally* update the underlying parameters for *on-policy* evaluation.

Policy evaluation with linear function approximation

Linear V/Q function approximation

The **value/Q** function is a *linear* combination of features:

$$V(s; w) = \phi(s)^\top w,$$

$$Q(s, a; w) = \psi(s, a)^\top v,$$

where

- $\phi(s)$ maps the state space $\mathcal{S}$ to $\mathbb{R}^{d_1}$;
- $\psi(s, a)$ maps the state-action space $\mathcal{S} \times \mathcal{A}$ to $\mathbb{R}^{d_2}$;
- w, v are the *low-dimensional embeddings* we wish to learn.

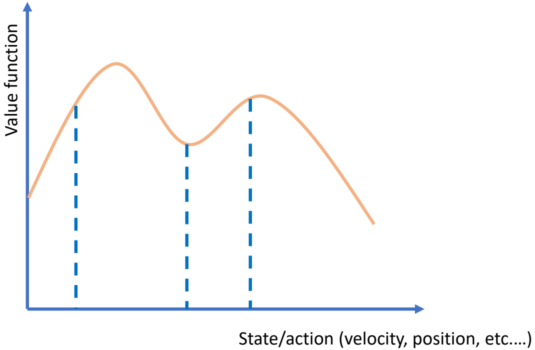
Typically, the number of features is much smaller than the dimension, i.e.

$$d_1 \ll |\mathcal{S}|, \qquad d_2 \ll |\mathcal{S}||\mathcal{A}|.$$

We assume the feature maps are **known**.

Feature selection

When the states/actions are numbers, function approximation for value functions bears familiarity with that of **interpolation and regression** in supervised learning.



Example features: polynomials, Fourier basis, radial basis functions,...

Incremental update with true value

Objective function:

$$J(w) = \frac{1}{2}\mathbb{E}_{s\sim d^\pi}\underbrace{\left[(V^\pi(s) - V(s;w))^2\right]}_{=:J(s;w)} = \frac{1}{2}\mathbb{E}_{s\sim d^\pi}\left[\left(V^\pi(s) - \phi(s)^\top w\right)^2\right],$$

which is *quadratic* w.r.t. w.

- Given access to $V^\pi(s)$, the stochastic gradient is evaluated as

$$\nabla_w J(s;w) = -\underbrace{\left(V^\pi(s) - \phi(s)^\top w\right)}_{\text{approx. error}}\phi(s).$$

- Update the weight w via

$$w \leftarrow w - \alpha\nabla_w J(s;w) = w + \alpha\left(V^\pi(s) - \phi(s)^\top w\right)\phi(s),$$

  where α is the learning rate.

Incremental update with target value

However, in reality, we do not have access to $V^\pi(s)$ (otherwise we won't need to learn!).

Instead: replace $V^\pi(s)$ by its target $V^\pi_{\text{target}}(s)$ from MC or TD.

$$J(w) = \frac{1}{2}\mathbb{E}_{s\sim d^\pi} \underbrace{\left[\left(V^\pi_{\text{target}}(s) - \phi(s)^\top w\right)^2\right]}_{=: J(s;w)},$$

Update the weight w via

$$w \leftarrow w - \alpha \nabla_w J(s;w) = w + \alpha \left(V^\pi_{\text{target}}(s) - \phi(s)^\top w\right) \phi(s),$$

where α is the learning rate.

Examples of different targets

- In MC, use the return G_t

$$w \leftarrow w + \alpha \left(G_t - \phi(s)^\top w \right) \phi(s)$$

- In TD(0), use the TD target $r_t + \gamma V(s_{t+1}, w) = r_t + \gamma \phi(s_{t+1})^\top w$

$$w \leftarrow w + \alpha \left(r_t + \gamma \phi(s_{t+1})^\top w - \phi(s_t)^\top w \right) \phi(s_t)$$

- In TD(λ), use the λ-return G_t^λ

$$w \leftarrow w + \alpha \left(G_t^\lambda - \phi(s)^\top w \right) \phi(s)$$

These are **“semi-gradient”** methods, since we only consider the gradient of the function approximator, not the target.

Convergence of TD(0) with linear function approximation

TD(0) with linear function approximation

Suppose we collect a trajectory following policy π:

$$s_0, r_0, s_1, r_1, s_2, r_2, \dots$$

TD(0) on a single trajectory:

$$w_{t+1} \leftarrow w_t + \alpha_t \left(r_t + \gamma \phi(s_{t+1})^\top w_t - \phi(s_t)^\top w_t \right) \phi(s_t)$$

Question

Does TD(0) converge on a single trajectory, and if so, what does it converge to? How does the choice of feature vectors impact performance?

Matrix representation

Feature matrix and reward vector: suppose $\mathcal{S}$ is finite with size S,

$$\Phi = [\phi(1), \phi(2), \ldots, \phi(S)]^\top = \begin{bmatrix} \phi(1)^\top \\ \phi(2)^\top \\ \vdots \\ \phi(S)^\top \end{bmatrix} \in \mathbb{R}^{S \times d}, \quad r = \begin{bmatrix} r(1) \\ r(2) \\ \vdots \\ r(S) \end{bmatrix} \in \mathbb{R}^S,$$

where we assume Φ is of **full column rank**.

Value function approximation: the value function is approximated as

$$V_w = \Phi w = [\phi(1), \phi(2), \ldots, \phi(S)]^\top w \in \mathsf{span}(\Phi).$$

Assumptions: the feature maps are bounded:

$$\|\phi(s)\|_2 \leq 1 \qquad\qquad \forall s \in \mathcal{S}$$

The TD(0) update rule in matrix form

The update rule of TD(0) can be written as

$$w_{t+1} = w_t - \alpha_t (A_t w_t - b_t)$$

where

$$\begin{aligned} A_t &= \phi(s_t)\big(\phi(s_t) - \gamma\phi(s_{t+1})\big)^\top \in \mathbb{R}^{d\times d}, \\ b_t &= \phi(s_t) r_t \in \mathbb{R}^d. \end{aligned}$$

Question

What is the fixed point of TD(0)?

Intuition: If we let $w_{t+1} = w_t$, then TD(0) should approximately solve the "average" version of this equation:

$$A_t w_t \approx b_t.$$

Stochastic approximation view of TD(0)

State stationary distribution μ of the Markov chain:

$$D_\mu = \begin{bmatrix} \mu(1) & & & \\ & \mu(2) & & \\ & & \ddots & \\ & & & \mu(S) \end{bmatrix},$$

and $\mu(s) > 0$ for all $s \in \mathcal{S}$.

Population version: averaging A_t and b_t over μ:

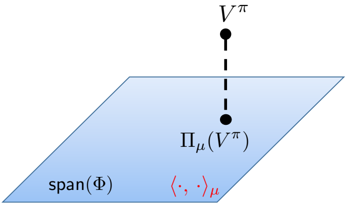
$$\mathbb{E}_{s_t \sim \mu}[A_t] = \Phi^\top D_\mu \big(I - \gamma P^\pi\big)\Phi := A \in \mathbb{R}^{d \times d}$$
$$\mathbb{E}_{s_t \sim \mu}[b_t] = \Phi^\top D_\mu r := b \in \mathbb{R}^{d}$$

TD(0) applies stochastic approximation to solve the linear system of equations:

$$Aw = b.$$

— but what is this, really?

Best linear function approximation to V^π?



A natural projection criteria is

$$\Pi_\mu(V^\pi) = \arg\min_{z=\Phi w} \sum_{s\in\mathcal{S}} \mu(s) \left(V^\pi(s) - \phi(s)^\top w\right)^2$$
$$= \arg\min_{z=\Phi w} \|V^\pi - \Phi w\|_\mu^2,$$

where we weigh the importance of different states by μ.

- The solution is

$$\Pi_\mu(V^\pi) = \Phi(\underbrace{\Phi^\top D_\mu \Phi}_{=:\Sigma})^{-1} \Phi^\top D_\mu V^\pi,$$

where Σ is the **covariance** w.r.t. the features weighted by μ:

$$\Sigma = \Phi^\top D_\mu \Phi = \mathbb{E}_{s\sim\mu}\left[\phi(s)\phi(s)^\top\right].$$

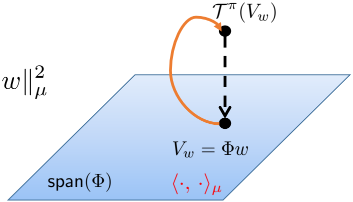
Projected Bellman equation

In TD(0), the target is the one-step look-ahead of $V_w = \Phi w$:

$$\mathcal{T}^\pi(\Phi w) = r + \gamma P^\pi \Phi w$$

Project this back to span(Φ):

$$\min_w \|\mathcal{T}^\pi(\Phi w) - \Phi w\|_\mu^2$$



Projected Bellman equation

$$\Phi w = \Pi_\mu \mathcal{T}(\Phi w)$$

where $\Pi_\mu(v) = \text{argmin}_{z \in \Phi w} \|z - v\|_\mu^2$.

Fixed-point of projected Bellman equation

The fixed-point of projected Bellman equation satisfies:

$$w = (\Phi^\top D_\mu \Phi)^{-1} \Phi^\top D_\mu (r + \gamma P^\pi \Phi w),$$

$$\Updownarrow$$

$$(\Phi^\top D_\mu \Phi) w = \Phi^\top D_\mu (r + \gamma P^\pi \Phi w)$$

$$\Updownarrow$$

$$\underbrace{\Phi^\top D_\mu (I - \gamma P^\pi) \Phi}_{=:A} w = \underbrace{\Phi^\top D_\mu r}_{=:b}$$

— TD(0) applies stochastic approximation to solve this!

Asymptotic convergence

Theorem 1 ([Tsitsiklis and Van Roy, 1997])

TD converges to the fixed point $w^\star$ of the projected Bellman equation

$$\Phi w = \Pi_\mu \mathcal{T}(\Phi w)$$

where $\Pi_\mu(v) = \textit{argmin}_{z\in\Phi w}\|z - v\|_\mu^2$, *as long*

$$\sum_{t=0}^{\infty} \alpha_t = \infty \quad \textit{and} \quad \sum_{t=0}^{\infty} \alpha_t^2 < \infty.$$

In addition,

$$\underbrace{\|V_{w^\star} - V^\pi\|_\mu}_{\textit{TD error}} \leq \frac{1}{(1-\gamma)} \underbrace{\|\Pi_\mu V^\pi - V^\pi\|_\mu}_{\textit{approx. error}}.$$

- asymptotic convergence
- approximation error

Proof

$$\underbrace{\|V_{w^\star} - V^\pi\|_\mu}_{\text{TD error}} \leq \frac{1}{(1-\gamma)} \underbrace{\|\Pi_\mu V^\pi - V^\pi\|_\mu}_{\text{approx. error}}.$$

Proof:

$$\begin{aligned}
&\|\Phi w^\star - V^\pi\|_\mu \\
&\leq \|\Phi w^\star - \Pi_\mu V^\pi\|_\mu + \|\Pi_\mu V^\pi - V^\pi\|_\mu && \text{(triangle inequality)} \\
&\leq \|\Pi_\mu \mathcal{T}(\Phi w^\star) - \Pi_\mu V^\pi\|_\mu + \|\Pi_\mu V^\pi - V^\pi\|_\mu && \text{(fixed point)} \\
&\leq \|\mathcal{T}(\Phi w^\star) - V^\pi\|_\mu + \|\Pi_\mu V^\pi - V^\pi\|_\mu && \text{(nonexpansiveness of } \Pi_\mu\text{)} \\
&\leq \|\mathcal{T}(\Phi w^\star) - \mathcal{T} V^\pi\|_\mu + \|\Pi_\mu V^\pi - V^\pi\|_\mu && \text{(Bellman equation)} \\
&\leq \gamma\|\Phi w^\star - V^\pi\|_\mu + \|\Pi_\mu V^\pi - V^\pi\|_\mu && \text{(Bellman contraction)}
\end{aligned}$$

Finite-time convergence of TD(0) with LFA

Polyak-Ruppert averaging: $$\overline{w}_T = \frac{1}{T}\sum_{i=1}^{T} w_i$$

Theorem 2 (Li*, Wu*, et al. 2023)

Under i.i.d. data, consider any $0 \le \delta \le 1$, *and* $0 < \epsilon \le \max\{1, \|w^\star\|_\Sigma\}$. *There exists some universal constant* $C > 0$ *such that*

$$\|\overline{w}_T - w^\star\|_\Sigma \le \epsilon$$

with probability at least $1-\delta$, *provided that the sample size exceeds*

$$T \ge C\frac{(\max_s \phi(s)^\top \Sigma^{-1}\phi(s))(1+\|w^\star\|_\Sigma^2)\log(d/\delta)}{(1-\gamma)^2\epsilon^2}.$$

Interpretation: when $\|w^\star\|_\Sigma^2 \ge 1$, ϵ-accuracy as soon as

$$T \gtrsim \frac{\kappa\|w^\star\|_2^2}{(1-\gamma)^2\epsilon^2}, \qquad \text{where} \quad \kappa = \frac{\lambda_{\max}(\Sigma)}{\lambda_{\min}(\Sigma)}.$$

Extensions

Least-squares TD (LSTD)

[Bradtke and Barto, 1996]: Given a collection of training data

$$(s_t, V^\pi(s_t)), \qquad t = 0, \ldots, T-1$$

We can also instead minimize the **batch** loss:

$$J(w) = \sum_{t=0}^{T-1} \left(V^\pi(s_t) - \phi(s_t)^\top w\right)^2$$

with the hope this leads to estimates with lower variance.

Step 1: Setting $\nabla_w J(w) = 0$, we have

$$\sum_{t=0}^{T-1} \left(V^\pi(s_t) - \phi(s_t)^\top w\right) \phi(s_t) = 0$$

Solution to LSTD

Step 2: Replace $V^\pi(s_t)$ by the target $r_t + \gamma\phi(s_{t+1})^\top w$ to obtain

$$\sum_{t=0}^{T-1} \left(r_t + \gamma\phi(s_{t+1})^\top w - \phi(s_t)^\top w\right) \phi(s_t) = 0.$$

$$\implies \quad w = \left(\sum_{t=0}^{T-1} \phi(s_t)(\phi(s_t) - \gamma\phi(s_{t+1}))^\top\right)^{-1} \left(\sum_{t=0}^{T-1} r_t\phi(s_t)\right).$$

- Recall

$$A_t = \phi(s_t)\big(\phi(s_t) - \gamma\phi(s_{t+1})\big)^\top \in \mathbb{R}^{d\times d}, \quad b_t = \phi(s_t)r_t \in \mathbb{R}^d.$$

- Aggregate the stochastic equations

$$\widehat{A} = \sum_{t=0}^{T-1} A_t = \sum_{t=0}^{T-1} \phi(s_t)\big(\phi(s_t) - \gamma\phi(s_{t+1})\big)^\top$$

$$\widehat{b} = \sum_{t=0}^{T-1} b_t = \sum_{t=0}^{T-1} \phi(s_t)r(s_t) \qquad \implies \qquad w = \widehat{A}^{-1}\widehat{b}$$

LSTD vs TD

$$\widehat{A} = \sum_{t=0}^{T-1} A_t = \sum_{t=0}^{T-1} \phi(s_t)\big(\phi(s_t) - \gamma\phi(s_{t+1})\big)^\top$$

$$\widehat{b} = \sum_{t=0}^{T-1} b_t = \sum_{t=0}^{T-1} \phi(s_t) r_t \qquad \Longrightarrow \qquad w = \widehat{A}^{-1}\widehat{b}$$

- Can be solved by direct calculation, or TD with experience replay.
- More sample efficient than TD.
- Computationally more expensive than TD, but can be made relatively efficient via recursive calculation by applying rank-one updates.

Beyond linear function approximation

Objective function:

$$J(w) = \frac{1}{2}\mathbb{E}_{s\sim d^\pi}\underbrace{\left[\left(V^\pi(s) - V(s;w)\right)^2\right]}_{=:J(s;w)},$$

where $V(s;w)$ is a differentiable function approximator.

- Given access to $V^\pi(s)$, the stochastic gradient is evaluated as

$$\nabla_w J(s;w) = \underbrace{\left(V^\pi(s) - V(s;w)\right)}_{\text{approx. error}}\nabla_w V(s;w).$$

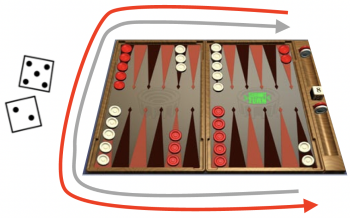
- Update the weight w via

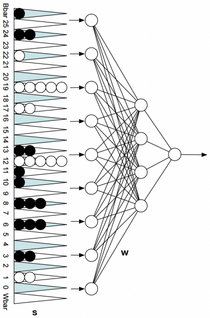
$$w \leftarrow w - \alpha\nabla_w J(s;w) = w + \alpha\left(V^\pi(s) - V(s;w)\right)\nabla_w V(s;w),$$

where α is the learning rate.

TD-Gammon

— [Tesauro, 1995]





- Value network: three-layer neural network
- Self-play: millions of games played against itself
- Beat the best human player of backgammon at the time

References I

Bradtke, S. J. and Barto, A. G. (1996).
Linear least-squares algorithms for temporal difference learning.
Machine learning, 22(1-3):33–57.

Tesauro, G. (1995).
Temporal difference learning and td-gammon.
Communications of the ACM, 38(3):58–68.

Tsitsiklis, J. and Van Roy, B. (1997).
An analysis of temporal-difference learning with function approximation.
IEEE Transactions on Automatic Control, 42(5):674–690.